

## SUPPLEMENTARY MATERIAL

### **Antitumour and Antimetastatic Effects and Safety Profile of a New Magnesium(II)-Chrysin Complex**

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It is possible to estimate the stability constant determining the dissociation degree  $\alpha$  of the complex using the following equation (1).

$$\alpha = \frac{A_m - A_s}{A_m} \quad (1)$$

$A_m$  and  $A_s$  are the absorbance of the solution containing an excess and stoichiometric amount of reagent, respectively. The stability constant can be calculated based on the following equation (2)

$$K_{st} = \frac{(1-\alpha)C}{(\alpha C)^2} \quad (2)$$

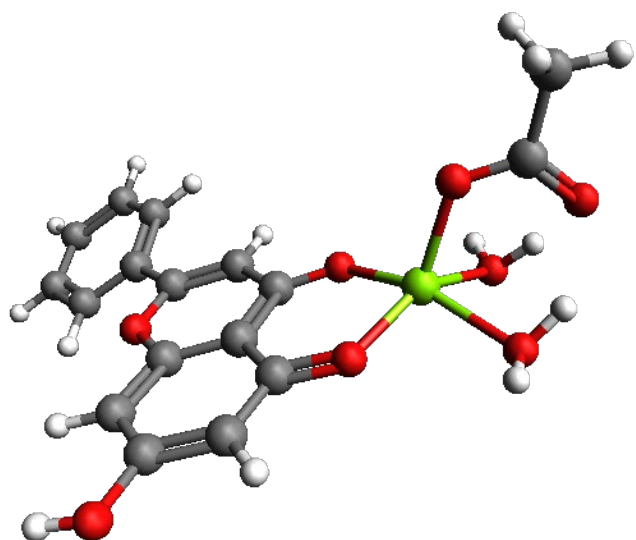
Table S1. Energy of Mgchrys conformers optimized in gas phase at B3LYP/6-31G\* and B3LYP/6-311++G\*\* theory levels. The major conformers at B3LYP/6-311++G\*\* theory level are in bold.

| Conformer        | B3LYP/6-31G* theory level |                         |                                  | B3LYP/6-311++G** theory level |                         |                                  |
|------------------|---------------------------|-------------------------|----------------------------------|-------------------------------|-------------------------|----------------------------------|
|                  | Energy <sup>a</sup>       | $\Delta E$ <sup>b</sup> | Relative population <sup>c</sup> | Energy <sup>a</sup>           | $\Delta E$ <sup>b</sup> | Relative population <sup>c</sup> |
| Mgchrys1         | -915689.0072              | 0.00                    | 10.41                            | -915943.0896                  | 0.63                    | 4.01                             |
| Mgchrys2         | -915688.9972              | 0.01                    | 10.14                            | -915943.0337                  | 0.68                    | 6.23                             |
| <b>Mgchrys3</b>  | -915688.8095              | 0.20                    | 11.38                            | <b>-915943.6838</b>           | <b>0.03</b>             | <b>10.92</b>                     |
| <b>Mgchrys4</b>  | -915688.6382              | 0.37                    | 10.37                            | <b>-915943.7083</b>           | <b>0.01</b>             | <b>9.97</b>                      |
| Mgchrys5         | -915688.4092              | 0.60                    | 9.89                             | -915943.0017                  | 0.71                    | 7.71                             |
| <b>Mgchrys6</b>  | -915688.1281              | 0.88                    | 8.98                             | <b>-915943.6882</b>           | <b>0.03</b>             | <b>11.22</b>                     |
| Mgchrys7         | -915687.9724              | 1.03                    | 7.24                             | -915941.8791                  | 1.84                    | 3.75                             |
| Mgchrys8         | -915687.9210              | 1.09                    | 8.12                             | -915942.2575                  | 1.46                    | 4.89                             |
| <b>Mgchrys9</b>  | -915687.3914              | 1.62                    | 6.44                             | <b>-915943.6700</b>           | <b>0.05</b>             | <b>12.11</b>                     |
| <b>Mgchrys10</b> | -915686.8461              | 2.16                    | 6.32                             | <b>-915943.7158</b>           | <b>0.00</b>             | <b>9.95</b>                      |
| <b>Mgchrys11</b> | -915686.7475              | 2.26                    | 5.20                             | <b>-915943.5238</b>           | <b>0.19</b>             | <b>12.19</b>                     |
| Mgchrys12        | -915686.6798              | 2.33                    | 5.50                             | -915942.6785                  | 1.04                    | 7.04                             |

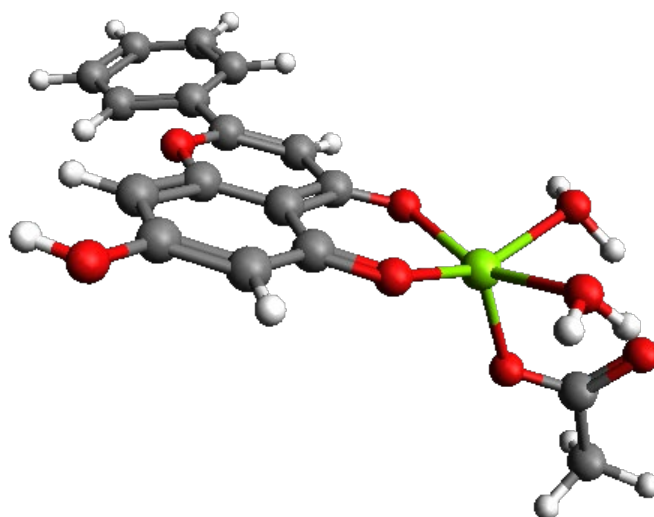
<sup>a</sup> Energy corrected by zero point energy (ZPE), expressed in kcal mol<sup>-1</sup>.

<sup>b</sup> Energy difference relative to the most stable conformer, expressed in kcal mol<sup>-1</sup>.

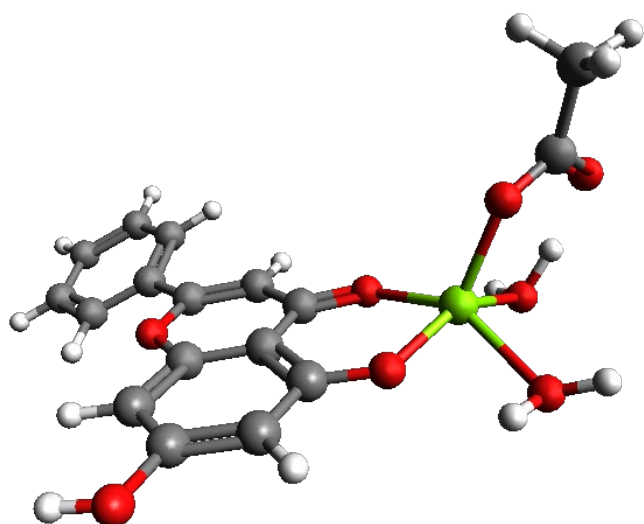
<sup>c</sup> Relative Population percentage calculated by Boltzmann, expressed in %.



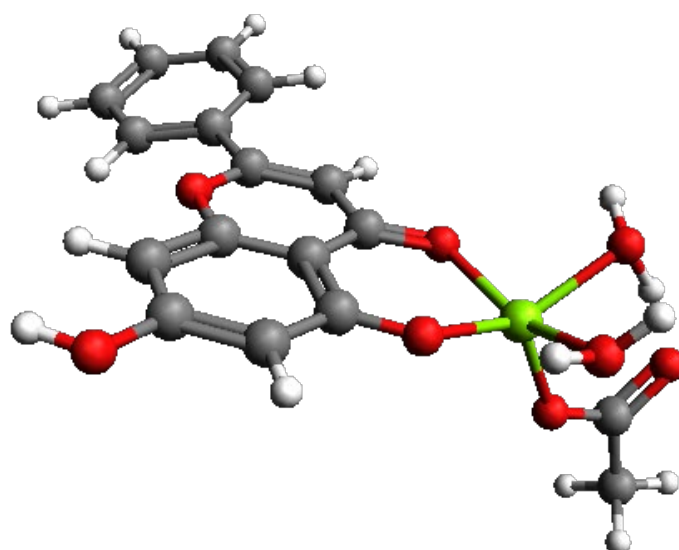
Mgchrys1



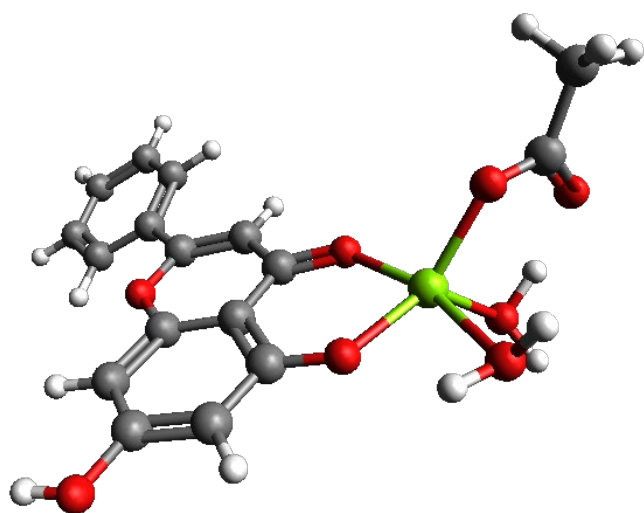
Mgchrys2



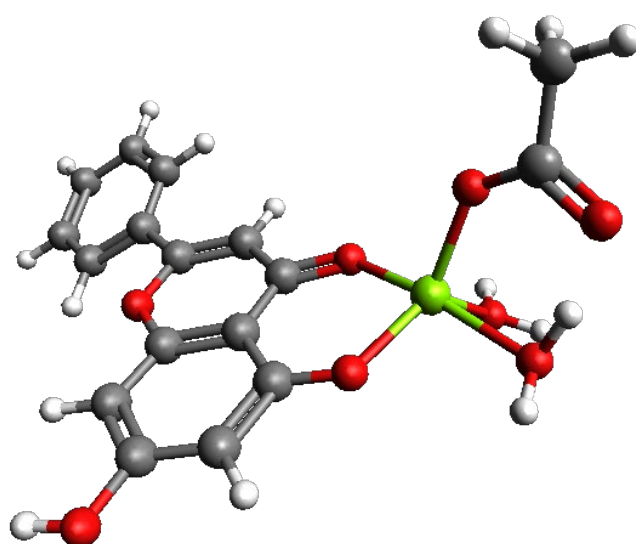
Mgchrys3



Mgchrys4



Mgchrys5



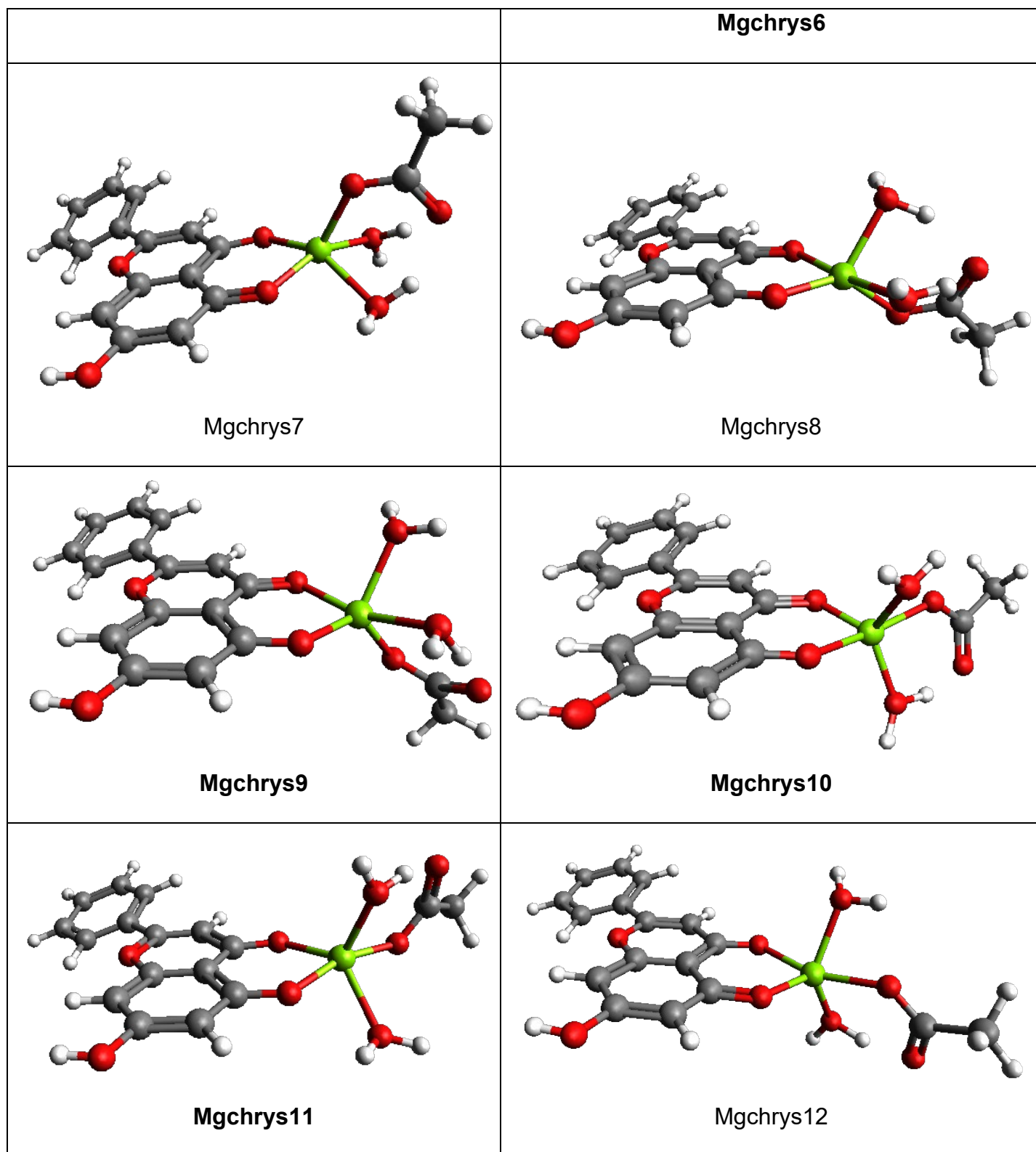


Figure. S1. Geometries of the twelve Mgchrys conformers optimized at B3LYP/6-311++G\*\* theory level with a  $\Delta E$  lower than 2 kcal mol<sup>-1</sup>. The major conformers of Mgchrys at B3LYP/6-311++G\*\* theory level attending the high stability and contribution percentages are in bold.

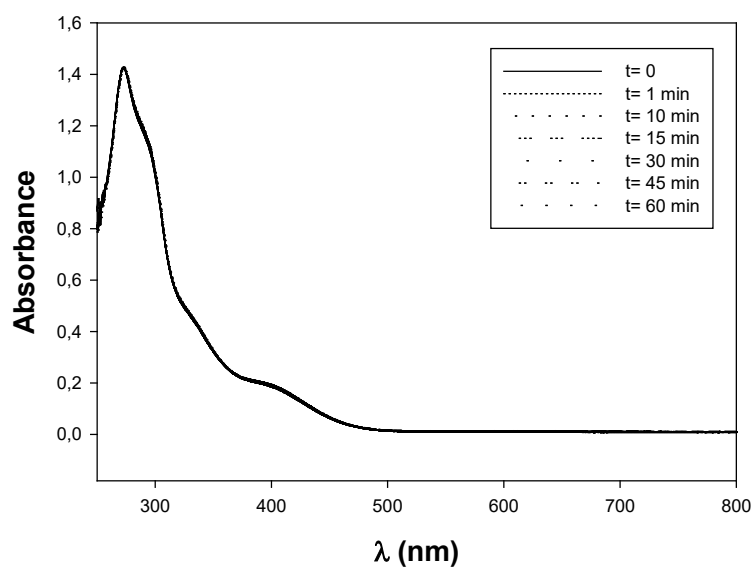


Figure S2. Electronic absorption spectra of Mgchrys in DMSO at different times (0, 1, 10, 15, 30, 45 and 60 minutes).

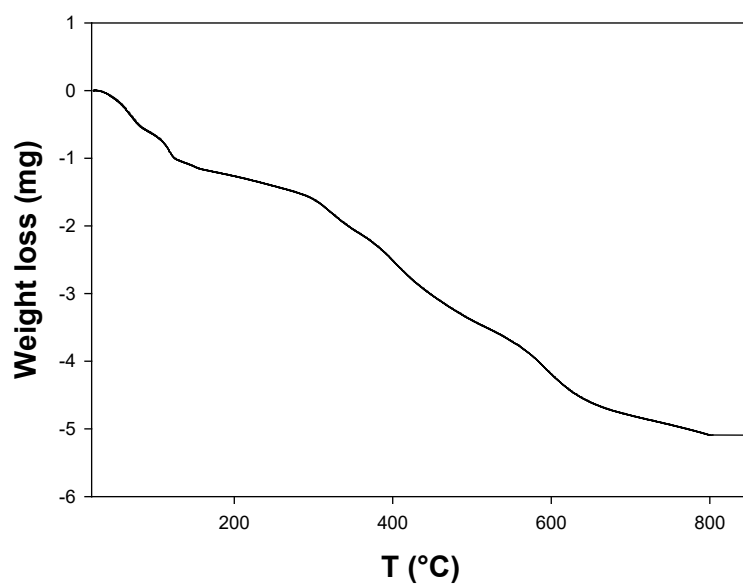


Figure S3. Thermogravimetric (TGA) curve of Mgchrys complex.

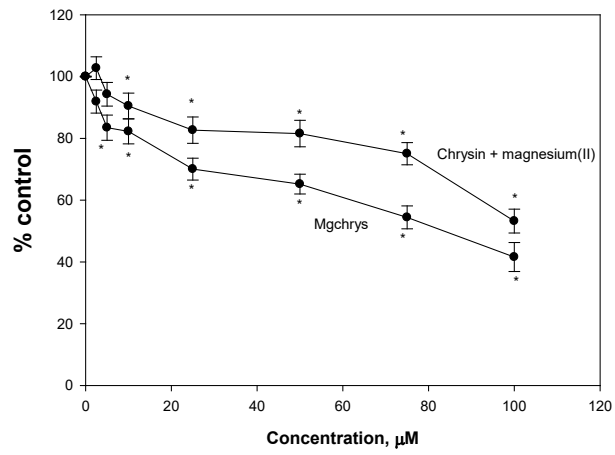


Figure S4. Effects of chrysin plus magnesium(II) cation and Mgchrys on A549 cell line viability. The results are expressed as the percentage of the control level and represent the mean  $\pm$  the standard error of the mean (SEM) from three separate experiments. \* significant values in comparison with the control level ( $p < 0.05$ ).